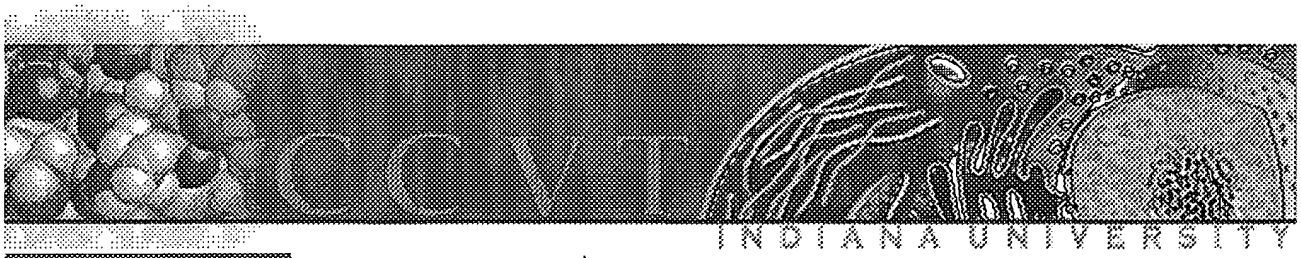

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Publications

Jaqaman, K. and P. Ortoleva. 2002. New space warping method for the simulation of large-scale macromolecular conformational changes, *Journal of Computational Chemistry*, Vol 23(1), 484-491.

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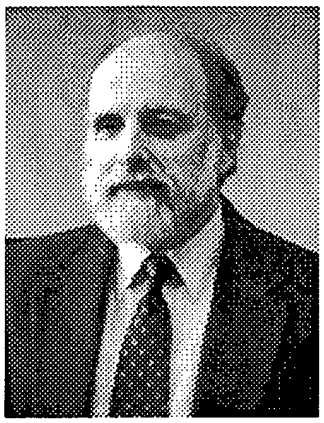
Peter Ortoleva



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Research

A unified approach to the modeling of a range of phenomena from intracrystalline zoning to basin diagenesis is adopted. The emphasis is on the challenging problem of strongly coupled systems.

Models are under development for oscillatory and sector crystal zoning, differentiated diagenetic and metamorphic layering, stylolites, banded and mosaic agates and temporally oscillatory fluid migration in sedimentary basins.

Petroleum and mineral exploration is being facilitated by the development of a basin diagenesis code which accounts for a complete suite of mechanical, reaction and transport processes. The code is used to predict the distribution of diagenetic and structural petroleum traps within the basin and the development of over- and under-pressures in reservoir rock. Another code focuses on the imposition of reactive fluids on a rock over geological or engineering time scales.

This research is supported by grants from the US DOE, Gas Research Institute, NSF, the EPA and the petroleum and computer industries. The Indiana University Laboratory for Computational Geochemistry under Ortoleva's supervision provides an interdisciplinary research environment and supports about 15 graduate and postdoctoral students from computer science, chemistry, geology, mathematics and physics, one half being from the Department of Geological Sciences.

Representative Publications

Meshri, I. and P. Ortoleva, eds., Prediction of Reservoir quality through chemical modeling: (1990). AAPG Memoir 49, 175p.

Ortoleva, P., B. Hallet, A. McBirney, I. Meshri, R. Reeder, and P. Williams, eds., Self- organization in geological systems: (1990). Proceedings of a workshop held 26-30 June 1988, University of California, Santa Barbara. Earth Science Reviews 29, Amsterdam, Elsevier, 417p.

Ortoleva, P., Nonlinear chemical waves: (1992). Chichester, John Wiley and Sons, 302p.

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Dewers, Thomas A. (Ph.D., 1990) Non-linear dynamics of coupled water-rock reaction, transport, and rock deformation.

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Payne, Dorothy F. (M.Sc., 1995) The effect of reaction-transport-mechanical processes on the spatial and temporal evolution of diagenetic phenomena in sedimentary basins: a test of the CIRFB code.

Sakrani, Khaireddine (Ph.D., 1996) A unified texture and mineralogy dependent model for rock deformation.

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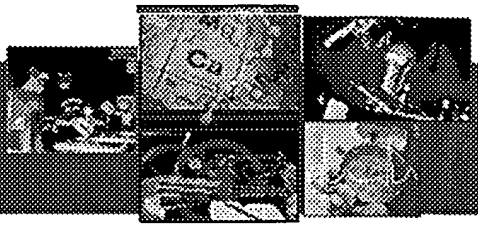
Faculty Publications

Chemistry Department



Indiana University Bloomington

Peter J. Ortoleva

Year-wise listing of Publications:

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2002

- Jaqaman, K. and Ortoleva, P. J. (2002). "New space warping method for the simulation of large-scale macromolecular conformational changes." Journal of Computational Chemistry **23**(4): 484-491.

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- Payne, D. F. and Ortoleva, P. J. (2001). "A model for lignin alteration - part II: numerical model of natural gas generation and application to the Piceance Basin, Western Colorado." Org. Geochem. **32**(9): 1087-1101.
- Payne, D. F. and Ortoleva, P. J. (2001). "A model for lignin alteration - part I: a kinetic reaction-network model." Org. Geochem. **32**(9): 1073-1085.
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- Ozkan, G. and Ortoleva, P. (2000). "A mesoscopic model of nucleation and Ostwald ripening/stepping. Application to the silica polymorph system." J. Chem. Phys. **112**(23): 10510-10525.
- Payne, D. F., Tuncay, K., Park, A., Comer, J. B. and Ortoleva, P. (2000). "A reaction-transport-mechanical approach to modeling the interrelationships among gas generation, overpressuring, and fracturing: implications for the Upper Cretaceous natural gas reservoirs of the Piceance Basin, Colorado." AAPG Bull. **84**(4): 545-565.

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Peter J. Ortoleva

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2004			
3	EE	Abdallah Sayyed-Ahmad, Kagan Tuncay, Peter J. Ortoleva: Efficient solution technique for solving the Poisson-Boltzmann equation. Journal of Computational Chemistry 25(8): 1068-1074 (2004)
2003			
2	EE	Elizabeth L. Weitzke, Peter J. Ortoleva: Simulating cellular dynamics through a coupled transcription, translation, metabolic model. Computational Biology and Chemistry 27(4-5): 469-480 (2003)
2002			
1	EE	Khuloud Jaqaman, Peter J. Ortoleva: New space warping method for the simulation of large-scale macromolecular conformational changes. Journal of Computational Chemistry 23(4): 484-491 (2002)

Coauthor Index

1	Khuloud Jaqaman	[1]
2	Abdallah Sayyed-Ahmad	[3]
3	Kagan Tuncay	[3]
4	Elizabeth L. Weitzke	[2]